Exact Gap between Generalization Error and Uniform Convergence in Random Feature Models

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Outline

- Problem Formulation
- Assumptions
- Main Theorem
- (Inferred) Asymptotic Power Laws
- Sketch of Proofs

Model setup

- Consider a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ with n samples.
- $\mathbf{x}_i \sim_{i.i.d.} \mathrm{Unif}(\mathbb{S}^{d-1}(\sqrt{d}))$ and $y_i = f_d(\mathbf{x}_i) + \epsilon_i$, where the noises $\epsilon_i \sim_{i.i.d.} \mathcal{N}(0, \tau^2)$ with $\tau^2 \geq 0$ are independent of $\{\mathbf{x}_i\}_{i=1}^n$.
- Let $(\boldsymbol{\theta}_j)_{j=1}^N \sim_{i.i.d.} \mathrm{Unif}\left(\mathbb{S}^{d-1}(\sqrt{d})\right)$.
- Given an activation function $\sigma : \mathbb{R} \to \mathbb{R}$, define the random features function class $\mathcal{F}_{\mathrm{RF}}(\boldsymbol{\Theta})$ by

$$\mathcal{F}_{\mathrm{RF}}(\boldsymbol{\Theta}) = \left\{ f(\mathbf{x}) = \sum_{j=1}^{N} a_j \sigma(\langle \mathbf{x}, \boldsymbol{\theta}_j \rangle / \sqrt{d}) : \boldsymbol{a} \in \mathbb{R}^N \right\}.$$

Generalization error and minimum norm interpolator

- Population risk: $R(\boldsymbol{a}) = \mathbb{E}_{\mathbf{x},y}\left(y - \sum_{j=1}^{N} a_j \sigma\left(\left\langle \mathbf{x}, \boldsymbol{\theta}_j \right\rangle / \sqrt{d}\right)\right)^2$.
- Empirical risk: $\hat{R}_n(\boldsymbol{a}) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{N} a_j \sigma\left(\left\langle \mathbf{x}_i, \boldsymbol{\theta}_j \right\rangle / \sqrt{d}\right)\right)^2$.
- Denote the regularized empirical risk minimizer with vanishing regularization by

$$\boldsymbol{a}_{\min} = \lim_{\lambda \to 0} \arg\min_{\boldsymbol{a}} \left[\hat{R}_n(\boldsymbol{a}) + \lambda \left\|\boldsymbol{a}\right\|_2^2\right].$$

- Note that $\hat{R}_n(\boldsymbol{a})$ is quadratic for random feature models and $\boldsymbol{a}_{\min}$ can be interpreted as the minimum ℓ_2 norm interpolator if $\min_{\boldsymbol{a}} \hat{R}_n(\boldsymbol{a}) = \hat{R}_n(\boldsymbol{a}_{\min}) = 0$, that is, $\boldsymbol{a}_{\min}$ is the solution to

$$\min_{\boldsymbol{a}} \left\|\boldsymbol{a}\right\|_2 \text{ s.t. } \hat{R}_n(\boldsymbol{a}) = 0$$

- Generalization error: $R(N, n, d) = R(\boldsymbol{a}_{\min})$.

Uniform convergence bounds

- Uniform convergence bound over a norm ball:

$$U(A, N, n, d) = \sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A} \left(R(\boldsymbol{a}) - \hat{R}_n(\boldsymbol{a}) \right).$$

- Uniform convergence over interpolators in the norm ball:

$$T(A, N, n, d) = \sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A, \hat{R}_n(\boldsymbol{a}) = 0} R(\boldsymbol{a}).$$

- We need $\hat{R}_n(\boldsymbol{a}_{\min}) = 0$ and take $A \ge (N/d)\|\boldsymbol{a}_{\min}\|_2^2$ to have a non-empty feasible region.
- For $A \ge (N/d)\|\boldsymbol{a}_{\min}\|$, there holds

$$U(A, N, n, d) \ge T(A, N, n, d) \ge R(\boldsymbol{a}_{\min}).$$

Assumptions

- **Assumption 1** (Linear target function). $f_d \in L^2\left(\mathbb{S}^{d-1}\left(\sqrt{d}\right)\right)$ with $f_d(\mathbf{x}) = \left\langle \boldsymbol{\beta}^{(d)}, \mathbf{x} \right\rangle$, where $\boldsymbol{\beta}^{(d)} \in \mathbb{R}^d$ and $\lim_{d\to\infty} \|\boldsymbol{\beta}^{(d)}\|_2^2 = F_1^2$.
- **Assumption 2** (Activation function). Let $\sigma \in C^2(\mathbb{R})$ with $|\sigma(u)|, |\sigma'(u)|, |\sigma''(u)| \leq c_0 e^{c_1|u|}$ for some constant $c_0, c_1 < \infty$. Define

$$\mu_0 = \mathbb{E}\left[\sigma(G)\right], \mu_1 = \mathbb{E}\left[G\sigma(G)\right], \mu_*^2 = \mathbb{E}\left[\sigma(G)^2\right] - \mu_0^2 - \mu_1^2,$$

  where the expectation is w.r.t. $G \sim \mathcal{N}(0,1)$. Assume $\mu_0 = 0$, $0 < \mu_1^2, \mu_*^2 < \infty$.
- **Assumption 3** (Proportional limit). Let $N = N(d)$ and $n = n(d)$. Assume that the following limits exist in $(0, \infty)$:

$$\lim_{d\to\infty} N/d = \psi_1, \lim_{d\to\infty} n/d = \psi_2.$$

- Other technical assumptions used in the proof.

Main Theorem

Theorem

Under Assumption 1, Assumption 2, Assumption 3, and other technical assumptions, there hold the following conclusions.

1. *For any* $A \in \Gamma_U$, *we have*

$$U(A, N, n, d) = \mathcal{U}(A, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1).$$

2. *For any* $A \in \Gamma_T$, *we have*

$$T(A, N, n, d) = \mathcal{T}(A, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1).$$

- Here the sets Γ_U and Γ_T will be defined later.
- The quantities $\mathcal{U}$ and $\mathcal{T}$ are involved and will be defined later.
- In a special case in this paper, the inferred asymptotic power law of $\mathcal{U}$ and $\mathcal{T}$ is given.

High dimensional regime

- In this paper, they consider the case where $d \to +\infty$.
- Denote $\hat{\psi}_1 = N/d$ and $\hat{\psi}_2 = n/d$. Recall the constrained $(N/d)\|\boldsymbol{a}\|_2^2 \leq A$ and the generalization error $R(\boldsymbol{a}_{\min})$.
- In addition to $\mathcal{U}$ and $\mathcal{T}$, Theorem 1 of Mei & Montanari (2019) implies the following convergence (in probability)

$$\hat{\psi}_1 \|\boldsymbol{a}_{\min}\|_2^2 \overset{d \to +\infty}{\longrightarrow} \mathcal{A}(\psi_1, \psi_2),$$
$$R(\boldsymbol{a}_{\min}) \overset{d \to +\infty}{\longrightarrow} \mathcal{R}(\psi_1, \psi_2).$$

- Here $\mathcal{A}$ and $\mathcal{R}$ are defined in Mei & Montanari (2019).

Kernel regime

- As $N \to \infty$, the random feature space $\mathcal{F}_{\mathrm{RF}}(\boldsymbol{\Theta})$ (equipped with proper inner product) converges to an RKHS (reproducing kernel Hilbert space) induce by the kernel

$$H(\mathbf{x}, \mathbf{x}') = \mathbb{E}_{\boldsymbol{\theta} \sim \mathrm{Unif}(\mathbb{S}^{d-1})} \left[\sigma\left(\langle \mathbf{x}, \boldsymbol{\theta} \rangle\right) \sigma\left(\langle \mathbf{x}', \boldsymbol{\theta} \rangle\right) \right].$$

- They expect that if they take $\psi_1 \to +\infty$ after $N, d, n \to +\infty$, the formula of $\mathcal{U}$ and $\mathcal{T}$ will coincide with the corresponding asymptotic limit of U and T for kernel ridge regression with the kernel H. (? an intuition)
- Denote

$$\mathcal{U}_\infty(A, \psi_2) = \lim_{\psi_1 \to \infty} \mathcal{U}(A, \psi_1, \psi_2), \quad \mathcal{T}_\infty(A, \psi_2) = \lim_{\psi_1 \to \infty} \mathcal{T}(A, \psi_1, \psi_2),$$
$$\mathcal{A}_\infty(\psi_2) = \lim_{\psi_1 \to +\infty} \mathcal{A}(\psi_1, \psi_2), \quad \mathcal{R}_\infty(\psi_2) = \lim_{\psi_1 \to \infty} \mathcal{R}(\psi_1, \psi_2).$$

Low norm uniform convergence bounds

- How to choose norm A in $\mathcal{U}$ and $\mathcal{T}$?
- We need at least $A \geq \hat{\psi}_1 \|\boldsymbol{a}_{\min}\|_2^2$. Therefore, we will choose

$$A = \alpha \hat{\psi}_1 \|\boldsymbol{a}_{\min}\|_2^2, \quad \text{for some } \alpha > 1.$$

- Note that $\hat{\psi}_1 \|\boldsymbol{a}_{\min}\|_2^2 \to \mathcal{A}(\psi_1, \psi_2)$ as $d \to +\infty$. For a fixed $\alpha > 1$, we further define

$$\mathcal{U}^{(\alpha)}(\psi_1, \psi_2) = \mathcal{U}(\alpha \mathcal{A}(\psi_1, \psi_2), \psi_1, \psi_2), \quad \mathcal{U}_\infty^{(\alpha)} = \lim_{\psi_1 \to \infty} \mathcal{U}^{(\alpha)}(\psi_1, \psi_2),$$

and

$$\mathcal{T}^{(\alpha)}(\psi_1, \psi_2) = \mathcal{T}(\alpha \mathcal{A}(\psi_1, \psi_2), \psi_1, \psi_2), \quad \mathcal{T}_\infty^{(\alpha)} = \lim_{\psi_1 \to \infty} \mathcal{T}^{(\alpha)}(\psi_1, \psi_2).$$

Inferred asymptotic power law, I

- Norm of the minimum norm interpolator:

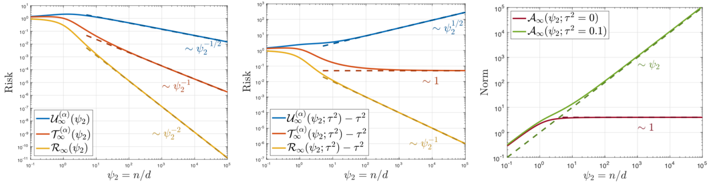
$$\mathcal{A}_\infty(\psi_2; \tau^2 > 0) \sim \psi_2, \quad \mathcal{A}_\infty(\psi_2; \tau^2 = 0) \sim 1.$$

- Kernel regime with noiseless data ($\tau^2 = 0$):

$$\mathcal{U}_\infty^{(\alpha)}(\psi_2) \sim \psi_2^{-1/2}, \quad \mathcal{T}_\infty^{(\alpha)} \sim \psi_2^{-1}, \quad \mathcal{R}_\infty(\psi_2) \sim \psi_2^{-2}.$$

- Kernel regime with noiseless data ($\tau^2 > 0$):

$$\mathcal{U}_\infty^{(\alpha)}(\psi_2) - \tau^2 \sim \psi_2^{1/2}, \quad \mathcal{T}_\infty^{(\alpha)} - \tau^2 \sim 1, \quad \mathcal{R}_\infty(\psi_2) - \tau^2 \sim \psi_2^{-1}.$$



(a) Noiseless response ($\tau^2 = 0$) (b) Noisy response ($\tau^2 = 0.1$) (c) Minimum norm $\mathcal{A}_\infty(\psi_2)$

Figure 1. Random feature regression with activation function $\sigma(x) = \max(0, x) - 1/\sqrt{2\pi}$, target function $f_d(\boldsymbol{x}) = \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle$ with $\|\boldsymbol{\beta}\|_2^2 = 1$, and $\psi_1 = \infty$. The horizontal axes are the number of samples $\psi_2 = \lim_{d\to\infty} n/d$. The solid lines are the the algebraic expressions derived in the main theorem (Theorem 1). The dashed lines are the function ψ_2^p in the log scale. Figure 1(a) and 1(b): Comparison of the classical uniform convergence in the norm ball of size level $\alpha = 1.5$ (Eq. (17), blue curve), the uniform convergence over interpolators in the same norm ball (Eq. (18), red curve), the risk of minimum norm interpolator (Eq. (13), yellow curve). Figure 1(c): Minimum norm required to interpolate the training data (Eq. (12)).

Inferred asymptotic power law, II

- The divergence of $\mathcal{U}_\infty^{(\alpha)}$ with noisy data is partly due to that $\mathcal{A}_\infty(\psi_2)$ blows up linearly in ψ_2.
- In fact, they can develop a heuristic intuition that $\mathcal{U}_\infty(A, \psi_2) \sim A/\psi_2^{1/2}$.

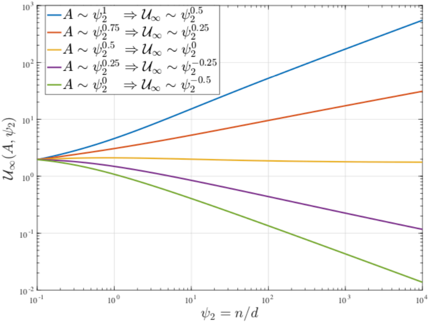


Figure 3. Uniform convergence $\mathcal{U}_\infty(A(\psi_2), \psi_2)$ over the norm ball in the kernel regime $\psi_1 \to \infty$. The size of the norm ball $A = A(\psi_2)$ is chosen according to different power laws as shown in the legend.

Inferred asymptotic power law, III

- Finite-width regime:

$$\mathcal{U}^{(\alpha)}(\psi_1,\psi_2) - \mathcal{U}_\infty^{(\alpha)}(\psi_2) \sim \psi_1^{-1},$$
$$\mathcal{T}^{(\alpha)}(\psi_1,\psi_2) - \mathcal{T}_\infty^{(\alpha)}(\psi_2) \sim \psi_1^{-1},$$
$$\mathcal{R}(\psi_1,\psi_2) - \mathcal{R}_\infty(\psi_2) \sim \psi_1^{-1},$$
$$\mathcal{A}(\psi_1,\psi_2) - \mathcal{A}_\infty(\psi_2) \sim \psi_1^{-1}.$$

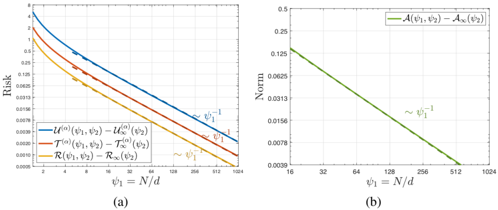


Figure 4. Random feature regression with the number of sample $\psi_2 = 1.5$, activation function $\sigma(x) = \max(0,x) - 1/\sqrt{2\pi}$, target function $f_d(\boldsymbol{x}) = \langle \boldsymbol{\beta}, \boldsymbol{x}\rangle$ with $\|\boldsymbol{\beta}\|_2^2 = 1$, and noise level $\tau^2 = 0.1$. The horizontal axes are the number of features ψ_1. The solid lines are the the algebraic expressions derived in the main theorem (Theorem 1). The dashed lines are the function ψ_1^p in the log scale. Figure 4(a): Comparison of the classical uniform convergence in the norm ball of size level $\alpha = 1.5$ (Eq. (15), blue curve), the uniform convergence over interpolators in the same norm ball (Eq. (16), red curve), the risk of minimum norm interpolator (Eq. (9), yellow curve). Figure 4(b): Minimum norm required to interpolate the training data (Eq. (8)).

Some notations

- Let $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$, $\mathbf{\Theta} = (\boldsymbol{\theta}_1, \cdots, \boldsymbol{\theta}_N)^\top \in \mathbb{R}^{N \times d}$, and $\mathbf{y} = (y_1, \cdots, y_n)^\top \in \mathbb{R}^n$.
- Denote $\mathbf{v} = (v_i)_{i \in [n]} \in \mathbb{R}^n$, $\mathbf{U} = (U_{ij})_{i,j \in [N]} \in \mathbb{R}^{N \times N}$, and $\mathbf{Z} = (Z_{ij})_{i \in [n], j \in [N]} \in \mathbb{R}^{n \times N}$ with

$$\begin{aligned} v_i &= \mathbb{E}_{\epsilon, \mathbf{x}} \left[y \sigma \left(\langle \mathbf{x}, \boldsymbol{\theta}_i \rangle / \sqrt{d} \right) \right], \\ U_{ij} &= \mathbb{E}_{\mathbf{x}} \left[\sigma \left(\langle \mathbf{x}, \boldsymbol{\theta}_i \rangle / \sqrt{d} \right) \sigma \left(\langle \mathbf{x}, \boldsymbol{\theta}_j \rangle / \sqrt{d} \right) \right], \\ Z_{ij} &= \sigma \left(\langle \mathbf{x}_i, \boldsymbol{\theta}_j \rangle / \sqrt{d} \right) / \sqrt{d}. \end{aligned}$$

- Rewrite

$$\begin{aligned} R(\boldsymbol{a}) &= \langle \boldsymbol{a}, \mathbf{U} \boldsymbol{a} \rangle - 2 \langle \boldsymbol{a}, \mathbf{v} \rangle + \mathbb{E}[y^2], \\ \hat{R}_n(\boldsymbol{a}) &= \frac{1}{n} \left\| \mathbf{y} - \sqrt{d} \mathbf{Z} \boldsymbol{a} \right\|_2^2 \\ &= \hat{\psi}_2^{-1} \langle \boldsymbol{a}, \mathbf{Z}^\top \mathbf{Z} \boldsymbol{a} \rangle - 2 \hat{\psi}_2^{-1} \frac{\langle \mathbf{Z}^\top \mathbf{y}, \boldsymbol{a} \rangle}{\sqrt{d}} + \frac{1}{n} \|\mathbf{y}\|_2^2. \end{aligned}$$

Strong duality

- Recall

$$U(A, N, n, d) = \sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A} \left(R(\boldsymbol{a}) - \hat{R}_n(\boldsymbol{a})\right),$$

$$T(A, N, n, d) = \sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A, \hat{R}_n(\boldsymbol{a})=0} R(\boldsymbol{a}).$$

- Let

$$\overline{U}(\lambda, N, n, d) = \sup_{\boldsymbol{a}} \left[R(\boldsymbol{a}) - \hat{R}_n(\boldsymbol{a}) - \hat{\psi}_1 \lambda \|\boldsymbol{a}\|_2^2\right],$$

$$\overline{T}(\lambda, N, n, d) = \sup_{\boldsymbol{a}} \inf_{\boldsymbol{\mu}} \left[R(\boldsymbol{a}) - \hat{\psi}_1 \lambda \|\boldsymbol{a}\|_2^2 + 2\left\langle \boldsymbol{\mu}, \mathbf{Z}\boldsymbol{a} - \mathbf{y}/\sqrt{d}\right\rangle\right].$$

Proposition 1

For any $A > 0$, there holds

$$U(A, N, n, d) = \inf_{\lambda \ge 0} \left[\overline{U}(\lambda, N, n, d) + \lambda A\right].$$

Moreover, for any $A > \hat{\psi}_1 \|\boldsymbol{a}_{\min}\|_2^2$, there holds

$$T(A, N, n, d) = \inf_{\lambda \ge 0} \left[\overline{T}(\lambda, N, n, d) + \lambda A\right].$$

Limit of dual forms

Proposition 2

Let assumptions in the main theorem hold. Then for $\lambda \in \Lambda_U$, with high probability the maximizer in the definition of $\overline{U}$ can be achieved at a unique point $\overline{\boldsymbol{a}}_U(\lambda)$ and we have

$$\begin{aligned}\overline{U}(\lambda, N, n, d) &= \overline{\mathcal{U}}(\lambda, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1), \\ \hat{\psi}_1 \|\overline{\boldsymbol{a}}_U(\lambda)\|_2^2 &= \mathcal{A}_U(\lambda, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1).\end{aligned}$$

Moreover, for $\lambda \in \Lambda_T$, with high probability the maximizer in the definition of $\overline{T}$ can be achieved at a unique point $\overline{\boldsymbol{a}}_T(\lambda)$ and we have

$$\begin{aligned}\overline{T}(\lambda, N, n, d) &= \overline{\mathcal{T}}(\lambda, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1), \\ \hat{\psi}_1 \|\overline{\boldsymbol{a}}_T(\lambda)\|_2^2 &= \mathcal{A}_T(\lambda, \psi_1, \psi_2) + o_{d,\mathbb{P}}(1).\end{aligned}$$

- The sets Λ_U and Λ_T will be given later in the proof.
- The definitions of $\overline{\mathcal{U}}, \overline{\mathcal{T}}, \mathcal{A}_U, \mathcal{A}_T$ are given in the appendix.

Heuristic formulae of quantities in Proposition 2

Remark 1. *Here we present the heuristic formulae of $\overline{\mathcal{U}}, \overline{\mathcal{T}}, \mathcal{A}_U, \mathcal{A}_T$, and defer their rigorous definition to the appendix. Define a function $g_0(\boldsymbol{q};\boldsymbol{\psi})$ by*

$$
\begin{aligned}
g_0(\boldsymbol{q};\boldsymbol{\psi}) \equiv\ & \mathrm{ext}_{z_1,z_2}\Big[\log\big((s_2z_1+1)(t_2z_2+1)\\
& -\mu_1^2(1+p)^2z_1z_2\big) - \mu_\star^2 z_1z_2 + s_1z_1 + t_1z_2 \\
& -\psi_1\log(z_1/\psi_1) - \psi_2\log(z_2/\psi_2) - \psi_1 - \psi_2\Big],
\end{aligned} \tag{22}
$$

where ext *stands for setting z_1 and z_2 to be stationery (which is a common symbol in statistical physics heuristics). We then take*

$$
\overline{\mathcal{U}}(\lambda,\boldsymbol{\psi}) = F_1^2(1-\mu_1^2\gamma_{s_2} - \gamma_p - \gamma_{t_2}) + \tau^2(1-\gamma_{t_1}),
$$

where $\gamma_a \equiv \partial_a g_0(\boldsymbol{q};\boldsymbol{\psi})|_{\boldsymbol{q}=(\mu_\star^2-\lambda\psi_1,\mu_1^2,\psi_2,0,0)}$ for the symbol $a \in \{s_1,s_2,t_1,t_2,p\}$, and

$$
\overline{\mathcal{T}}(\lambda,\boldsymbol{\psi}) = F_1^2(1-\mu_1^2\nu_{s_2} - \nu_p - \nu_{t_2}) + \tau^2(1-\nu_{t_1}),
$$

where we define $\nu_a \equiv \partial_a g_0(\boldsymbol{q};\boldsymbol{\psi})|_{\boldsymbol{q}=(\mu_\star^2-\lambda\psi_1,\mu_1^2,0,0,0)}$ for symbols $a \in \{s_1,s_2,t_1,t_2,p\}$. Finally $\mathcal{A}_U = -\partial_\lambda\overline{\mathcal{U}}$, $\mathcal{A}_T = -\partial_\lambda\overline{\mathcal{T}}$. By a further simplification, we can express these formulae to be rational functions of $(\mu_1^2,\mu_\star^2,\lambda,\psi_1,\psi_2,m_1,m_2)$ where (m_1,m_2) is the stationery point of the variational problem in Eq. (22) (c.f. Remark 2).

- Here $\mathbf{q} = (s_1,s_2,t_1,t_2,p)$ and $\boldsymbol{\psi} = (\psi_1,\psi_2)$.

Formulae for uniform convergence bounds

- For $A \in \Gamma_U = \{\mathcal{A}_U(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_U\}$, define

$$\mathcal{U}(A, \psi_1, \psi_2) = \inf_{\lambda \geq 0} \left[\overline{\mathcal{U}}(\lambda, \psi_1, \psi_2) + \lambda A \right].$$

- For $A \in \Gamma_T = \{\mathcal{A}_T(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_T\}$, define

$$\mathcal{T}(A, \psi_1, \psi_2) = \inf_{\lambda \geq 0} \left[\overline{\mathcal{T}}(\lambda, \psi_1, \psi_2) + \lambda A \right].$$

Key point of the proof of Proposition 1

- Strong duality holds for quadratic program with single quadratic constraint.
- For U, there holds

$$\sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A} \left(R(\boldsymbol{a}) - \hat{R}_n(\boldsymbol{a}) \right) = \inf_{\lambda \ge 0} \sup_{\boldsymbol{a}} \left[R(\boldsymbol{a}) - \hat{R}_n(\boldsymbol{a}) - \lambda \left(\hat{\psi}_1 \|\boldsymbol{a}\|_2^2 - A \right) \right].$$

- $\{\boldsymbol{a} : \hat{R}_n(\boldsymbol{a}) = 0\} = \{\boldsymbol{a}_{\min} + \mathbf{R}\mathbf{u}, \mathbf{u} \in \mathbb{R}^m\}$, where $m = \dim(\mathrm{Null}(\mathbf{Z}))$ and $\mathbf{R} \in \mathbb{R}^{N \times m}$ is a matrix such that $\mathrm{Span}(\mathbf{R}) = \mathrm{Null}(\mathbf{Z})$.
- There holds

$$\begin{aligned}
&\sup_{(N/d)\|\boldsymbol{a}\|_2^2 \le A,\, \hat{R}_n(\boldsymbol{a})=0} R(\boldsymbol{a}) \\
=& R(\boldsymbol{a}_{\min}) + \sup_{\|\mathbf{R}\mathbf{u} + \boldsymbol{a}_{\min}\|_2^2 \le \hat{\psi}_1^{-1} A} \left[\langle \mathbf{u}, \mathbf{R}^\top \mathbf{U} \mathbf{R} \mathbf{u} \rangle + 2 \langle \mathbf{R}\mathbf{u}, \mathbf{U}\boldsymbol{a}_{\min} - \mathbf{v} \rangle \right] \\
=& \inf_{\lambda \ge 0} \left\{ \lambda A + \sup_{\hat{R}_n(\boldsymbol{a})=0} \left[R(\boldsymbol{a}) - \lambda \hat{\psi}_1 \|\boldsymbol{a}\|_2^2 \right] \right\}
\end{aligned}$$

Proof sketch of Proposition 2

- The definitions of $\overline{U}$ and $\overline{T}$ depend on $\boldsymbol{\beta} = \boldsymbol{\beta}^{(d)}$ such that $f_d(\mathbf{x}) = \left\langle \boldsymbol{\beta}^{(d)}, \mathbf{x} \right\rangle$.
- Since $\mathbf{x}_i's$ ans $\boldsymbol{\theta}_i's$ are rotationally invariant, there holds $\overline{U}(\boldsymbol{\beta}_1, \lambda, N, n, d)$ $= \overline{U}(\boldsymbol{\beta}_2, \lambda, N, n, d)$ and $\overline{T}(\boldsymbol{\beta}_1, \lambda, N, n, d) = \overline{T}(\boldsymbol{\beta}_2, \lambda, N, n, d)$ for $\|\boldsymbol{\beta}_1\|_2 = \|\boldsymbol{\beta}_2\|_2$.
- In the proof, they work with the assumption that $\boldsymbol{\beta}^{(d)} \sim \mathrm{Unif}(\mathbb{S}^{d-1}(F_1))$.

Proof sketch of Proposition 2

- Recall the matrix $\mathbf{U} \in \mathbb{R}^{N\times N}$ with $U_{ij} = \mathbb{E}_{\mathbf{x}}\left[\sigma\left(\langle \mathbf{x}, \boldsymbol{\theta}_i\rangle / \sqrt{d}\right)\sigma\left(\langle \mathbf{x}, \boldsymbol{\theta}_j\rangle / \sqrt{d}\right)\right].$
- Let $\mathbf{Q} = \boldsymbol{\Theta}\boldsymbol{\Theta}^\top / d$ and let μ_1, μ_* be defined in Assumption 2.
- There holds the following decomposition

$$\mathbf{U} = \mu_1^2 \mathbf{Q} + \mu_*^2 \mathbf{I}_N + \boldsymbol{\Delta}$$

  with $\boldsymbol{\Delta}$ being a perturbation such that $\mathbb{E}[\|\boldsymbol{\Delta}\|_{\mathrm{op}}^2] = o_d(1)$.
- This decomposition was first proved by El Karoui (2010) for the Gaussian case and has been widely used in studying the interpolation regime (c.f., Liang & Rakhlin, 2020).
- Nonlinear $\to$ linear in high dimensions ($d \to +\infty$ (e.g.,this paper) or sufficiently large d (e.g., Liang & Rakhlin, 2020)).
- This decomposition requires the smoothness of σ.

Proof sketch of Proposition 2

In the following, we would like to show that $\boldsymbol{\Delta}$ has vanishing effects in the asymptotics of $\overline{U}$, $\overline{T}$, $\|\overline{\boldsymbol{a}}_U\|_2^2$ and $\|\overline{\boldsymbol{a}}_T\|_2^2$. For this purpose, we denote

$$\begin{aligned}
\boldsymbol{U}_c &= \mu_1^2 \boldsymbol{Q} + \mu_\star^2 \mathbf{I}_N, \\
R_c(\boldsymbol{a}) &= \langle \boldsymbol{a}, \boldsymbol{U}_c \boldsymbol{a} \rangle - 2\langle \boldsymbol{a}, \boldsymbol{v} \rangle + \mathbb{E}[y^2], \\
\widehat{R}_{c,n}(\boldsymbol{a}) &= \langle \boldsymbol{a}, \psi_2^{-1} \boldsymbol{Z}^\mathsf{T} \boldsymbol{Z} \boldsymbol{a} \rangle - 2\langle \boldsymbol{a}, \psi_2^{-1} \boldsymbol{Z}^\mathsf{T} \boldsymbol{y}/\sqrt{d} \rangle + \mathbb{E}[y^2], \\
\overline{U}_c(\lambda, N, n, d) &= \sup_{\boldsymbol{a}} \Big(R_c(\boldsymbol{a}) - \widehat{R}_{c,n}(\boldsymbol{a}) - \psi_1 \lambda \|\boldsymbol{a}\|_2^2 \Big), \\
\overline{T}_c(\lambda, N, n, d) &= \sup_{\boldsymbol{a}} \inf_{\boldsymbol{\mu}} \Big[R_c(\boldsymbol{a}) - \lambda \psi_1 \|\boldsymbol{a}\|_2^2 + 2\langle \boldsymbol{\mu}, \boldsymbol{Z}\boldsymbol{a} - \boldsymbol{y}/\sqrt{d} \,\rangle \Big].
\end{aligned}$$

- In the notations defined above, ψ_1 and ψ_2 should be $\hat{\psi}_1$ and $\hat{\psi}_2$, respectively.
- There holds

$$\overline{U}_c(\lambda, N, n, d) = \sup_{\boldsymbol{a}} \left(\left\langle \boldsymbol{a}, \overline{\mathbf{M}} \boldsymbol{a} \right\rangle - 2 \left\langle \boldsymbol{a}, \overline{\mathbf{v}} \right\rangle \right)$$

with $\overline{\mathbf{M}} = \mathbf{U}_c - \hat{\psi}_2^{-1} \mathbf{Z}^\top \mathbf{Z} - \hat{\psi}_1 \lambda \mathbf{I}_N$ and $\overline{\mathbf{v}} = \mathbf{v} - \hat{\psi}_2^{-1} \mathbf{Z}^\top \mathbf{y}/\sqrt{d}$.

Proof sketch of Proposition 2

- Assume that there exists $\delta > 0$ and $\lambda_U = \lambda_U(\psi_1, \psi_2, \mu_1^2, \mu_*^2)$ such that for any fixed $\lambda \in \Lambda_U = (\lambda_U, +\infty)$, there holds

$$\overline{\mathbf{M}} = \overline{\mathbf{M}}(\lambda) \preccurlyeq -\delta \mathbf{I}_N.$$

- For $\lambda \in \Lambda_U$, there holds $\overline{\boldsymbol{a}}_{U,c}(\lambda) = \overline{\mathbf{M}}^{-1} \overline{\mathbf{v}}$.
- Note that $\|\boldsymbol{\Delta}\|_{\mathrm{op}} = o_{d,\mathbb{P}}(1)$ and $\|\boldsymbol{\Delta}\|_{\mathrm{op}} \leq \delta/2$ with high probability for d large enough.
- $\overline{\boldsymbol{a}}_U(\lambda) = \left(\overline{\mathbf{M}} + \boldsymbol{\Delta}\right)^{-1} \overline{\mathbf{v}}$ for $\lambda \in \Lambda_U$ and d large enough.
- They have

$$\begin{aligned} \|\overline{\boldsymbol{a}}_U(\lambda)\|_2^2 &= (1 + o_{d,\mathbb{P}}) \left\|\overline{\boldsymbol{a}}_{U,c}(\lambda)\right\|_2^2, \\ \overline{U}_c(\lambda, N, n, d) &= \overline{U}(\lambda, N, n, d) + o_{d,\mathbb{P}} \left(\left\|\overline{\boldsymbol{a}}_{U,c}(\lambda)\right\|_2^2 + 1 \right). \end{aligned}$$

Proof sketch of Proposition 2

By Eq. (37) and (38), simple calculation shows that

$$\overline{U}_c(\lambda, N, n, d) \equiv -\langle \overline{\boldsymbol{v}}, \overline{\boldsymbol{M}}^{-1} \overline{\boldsymbol{v}} \rangle = -\Psi_1 - \Psi_2 - \Psi_3,$$
$$\|\overline{\boldsymbol{a}}_{U,c}\|_2^2 \equiv \langle \overline{\boldsymbol{v}}, \overline{\boldsymbol{M}}^{-2} \overline{\boldsymbol{v}} \rangle = \Phi_1 + \Phi_2 + \Phi_3,$$

where

$$\Psi_1 = \langle \boldsymbol{v}, \overline{\boldsymbol{M}}^{-1} \boldsymbol{v} \rangle, \qquad \Phi_1 = \langle \boldsymbol{v}, \overline{\boldsymbol{M}}^{-2} \boldsymbol{v} \rangle,$$
$$\Psi_2 = -2\psi_2^{-1} \langle \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}}, \overline{\boldsymbol{M}}^{-1} \boldsymbol{v} \rangle, \qquad \Phi_2 = -2\psi_2^{-1} \langle \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}}, \overline{\boldsymbol{M}}^{-2} \boldsymbol{v} \rangle,$$
$$\Psi_3 = \psi_2^{-2} \langle \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}}, \overline{\boldsymbol{M}}^{-1} \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}} \rangle, \qquad \Phi_3 = \psi_2^{-2} \langle \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}}, \overline{\boldsymbol{M}}^{-2} \frac{\boldsymbol{Z}^\top \boldsymbol{y}}{\sqrt{d}} \rangle.$$

- Here ψ_1 (ψ_2) should be $\hat{\psi}_1$ ($\hat{\psi}_2$).

Proof sketch of Proposition 2

Proposition 5. *Follow the assumptions of Proposition 2. For any $\lambda \in \Lambda_U$, denote $\boldsymbol{q}_U(\lambda, \boldsymbol{\psi}) = (\mu_\star^2 - \lambda\psi_1, \mu_1^2, \psi_2, 0, 0)$, then we have*

$$\begin{aligned}
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_1] \xrightarrow{\mathbb{P}} \mu_1^2 F_1^2 \cdot \partial_{s_2} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}),\\
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_2] \xrightarrow{\mathbb{P}} F_1^2 \cdot \partial_p g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}),\\
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_3] \xrightarrow{\mathbb{P}} F_1^2 \cdot \Big(\partial_{t_2} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}) - 1\Big) + \tau^2 \Big(\partial_{t_1} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}) - 1\Big),\\
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_1] \xrightarrow{\mathbb{P}} -\mu_1^2 F_1^2 \cdot \partial_{s1}\partial_{s2} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}),\\
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_2] \xrightarrow{\mathbb{P}} -F_1^2 \cdot \partial_{s1}\partial_p g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}),\\
&\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_3] \xrightarrow{\mathbb{P}} -F_1^2 \cdot \partial_{s_1}\partial_{t_2} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}) - \tau^2 \cdot \partial_{s_1}\partial_{t_1} g(0_+; \boldsymbol{q}_U(\lambda, \boldsymbol{\psi}); \boldsymbol{\psi}),
\end{aligned}$$

where $\nabla_{\boldsymbol{q}}^k g(0_+; \boldsymbol{q}; \boldsymbol{\psi})$ for $k \in \{1, 2\}$ stands for the k'th derivatives (as a vector or a matrix) of $g(\boldsymbol{i}u; \boldsymbol{q}; \boldsymbol{\psi})$ with respect to $\boldsymbol{q}$ in the $u \to 0+$ limit (with its elements given by partial derivatives)

$$\nabla_{\boldsymbol{q}}^k g(0_+; \boldsymbol{q}; \boldsymbol{\psi}) = \lim_{u \to 0_+} \nabla_{\boldsymbol{q}}^k g(\boldsymbol{i}u; \boldsymbol{q}; \boldsymbol{\psi}).$$

As a consequence, we have

$$\mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\overline{U}_c(\lambda, N, n, d)] \xrightarrow{\mathbb{P}} \overline{\mathcal{U}}(\lambda, \psi_1, \psi_2), \qquad \mathbb{E}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\psi_1 \|\overline{\boldsymbol{a}}_{U,c}(\lambda)\|_2^2] \xrightarrow{\mathbb{P}} \mathcal{A}_U(\lambda, \psi_1, \psi_2),$$

where the definitions of $\overline{\mathcal{U}}$ and $\mathcal{A}_U$ are given in Definition 5. Here $\xrightarrow{\mathbb{P}}$ stands for convergence in probability as $N/d \to \psi_1$ and $n/d \to \psi_2$ (with respect to the randomness of $\boldsymbol{X}$ and $\boldsymbol{\Theta}$).

- The idea of the proof of Proposition 5 follows mainly (Mei & Montanari, 2019)

Proof sketch of Proposition 2

Lemma 2. *Follow the assumptions of Proposition 2. For any $\lambda \in \Lambda_U$, we have*

$$\mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_1], \mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_2], \mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Psi_3] = o_{d,\mathbb{P}}(1),$$
$$\mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_1], \mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_2], \mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\Phi_3] = o_{d,\mathbb{P}}(1),$$

so that

$$\mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\overline{U}_c(\lambda, N, n, d)], \mathit{Var}_{\boldsymbol{\varepsilon},\boldsymbol{\beta}}[\|\overline{\boldsymbol{a}}_{U,c}(\lambda)\|_2^2] = o_{d,\mathbb{P}}(1).$$

Here, $o_{d,\mathbb{P}}(1)$ stands for converges to 0 in probability (with respect to the randomness of $\boldsymbol{X}$ and $\boldsymbol{\Theta}$) as $N/d \to \psi_1$ and $n/d \to \psi_2$ and $d \to \infty$.

Now, combining Lemma 2 and Proposition 5, we have

$$\overline{U}_c(\lambda, N, n, d) \xrightarrow{\mathbb{P}} \overline{\mathcal{U}}(\lambda, \psi_1, \psi_2), \quad \psi_1 \|\overline{\boldsymbol{a}}_{U,c}(\lambda)\|_2^2 \xrightarrow{\mathbb{P}} \mathcal{A}_U(\lambda, \psi_1, \psi_2),$$

Proof sketch of Proposition 2

- The proof of the results of T is similar to the proof of U by replacing $\overline{\mathbf{M}}$ and $\overline{\mathbf{v}}$ with $\widetilde{\mathbf{M}}$ and $\tilde{\mathbf{v}}$, accordingly. Here

$$\widetilde{\mathbf{M}} = \begin{bmatrix} \mathbf{U}_c - \hat{\psi}_1 \lambda \mathbf{I}_N & \mathbf{Z}^\top \\ \mathbf{Z} & \mathbf{0} \end{bmatrix}, \quad \tilde{\mathbf{v}} = \begin{bmatrix} \mathbf{v} \\ \mathbf{y}/\sqrt{d} \end{bmatrix}.$$

- Let $\mathbf{P}_{\mathrm{Null}} = \mathbf{I}_N - \mathbf{Z}^\dagger \mathbf{Z}$ be the projection onto $\mathrm{Null}(\mathbf{Z})$. Assume that there exists $\delta > 0$ and $\lambda_T = \lambda_T(\psi_1, \psi_2, \mu_1^2, \mu_*^2)$ such that for any fixed $\lambda \in \Lambda_T = (\lambda_T, \infty)$, there holds

$$\mathbf{P}_{\mathrm{Null}} \left[\mu_1^2 \mathbf{Q} + (\mu_*^2 - \hat{\psi}_1 \lambda) \mathbf{I}_N \right] \mathbf{P}_{\mathrm{Null}} \preccurlyeq -\delta \mathbf{P}_{\mathrm{Null}},$$

  and $\mathbf{Z}$ has full rank with $\sigma_{\min}(\mathbf{Z}) \geq \delta$.
- $\widetilde{\mathbf{M}} = \widetilde{\mathbf{M}}(\lambda)$ is invertible for $\lambda \in \Lambda_T$.

Proof sketch of the main theorem

- For $A \in \Gamma_U = \{\mathcal{A}_U(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_U\}$, we have

  $$\lambda_* = \lambda_*(A) = \inf_{\lambda} \{\lambda : \mathcal{A}_U(\lambda, \psi_1, \psi_2) = A\} \in \operatorname{Arg}\min_{\lambda \geq 0} \left[\overline{\mathcal{U}}(\lambda, \psi_1, \psi_2) + \lambda A\right].$$

  (easy to see?)
- $\overline{\mathcal{U}}(\lambda_*, \psi_1, \psi_2) + \lambda_* A = \mathcal{U}(A, \psi_1, \psi_2)$.
- $U(A, N, n, d) \leq \overline{U}(\lambda_*, N, n, d) + \lambda_* A$ (primal $\leq$ dual for max problem)
- $U(A + \delta, N, n, d) \geq \overline{U}(\lambda_*, N, n, d) + \lambda_*(A - \delta)$ for any $\delta > 0$ with high probability.

Thank You!